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# Chemistry Based Modeling of LLM-105 Explosives

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Chemistry Based Modeling of LLM-105 Explosives  
Aldermaston, United Kingdom  
May 18, 2015 through May 22, 2015

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## (U) Chemistry Based Modeling of LLM-105 Explosives



**JOWOG 9 Plenary Meeting**

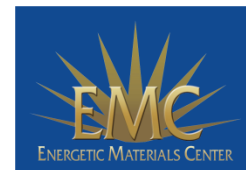
**AWE**

**May 18-22 2015**

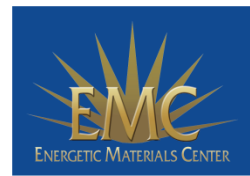
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**Energetic Material Center  
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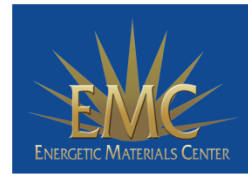
# LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide) is a newly developed insensitive high explosive with performance between that of HMX and TATB



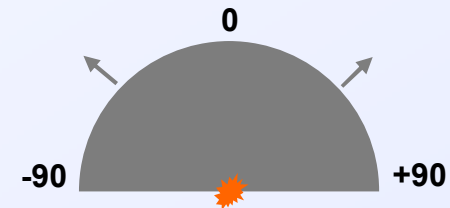
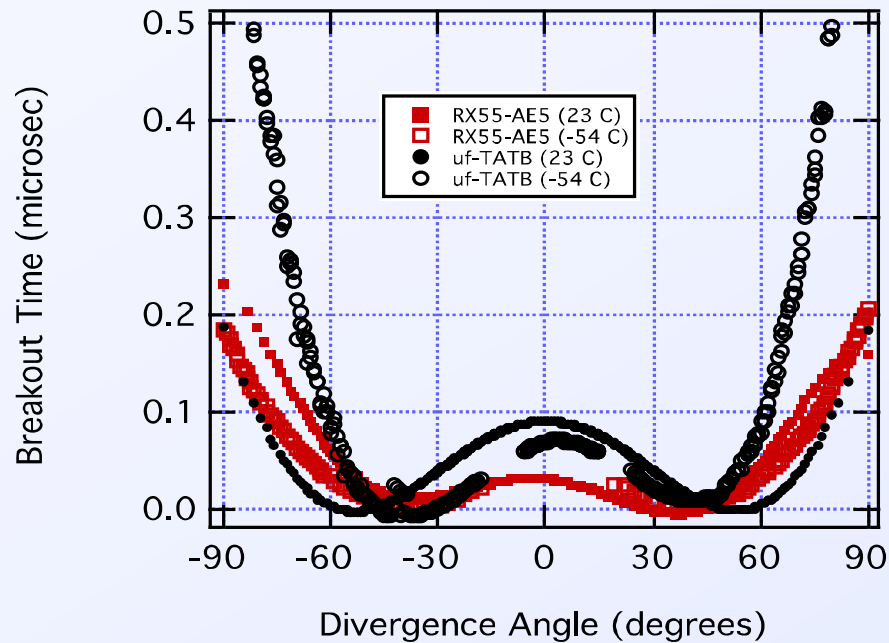
- LLM-105 is high-performance Insensitive High Explosive (IHE) material, attractive for applications that require moderate performance and insensitivity.
- Its calculated energy content is about 85% that of HMX and 15% more than that of TATB.
- It has excellent thermal stability and cold-performance behavior.
- It is insensitive to shock, spark and friction and has an impact insensitivity level approaching that of TATB.
- Changing synthesis and manufacturing paths have led to a variety of research formulations being developed at LLNL.
- Most all of the formulations have been PBX's - plastic bonded explosives.
- The LLNL research formulations have attempted to balance energy content with good compaction qualities, by varying the type and amount of binder Viton and Kel-F.



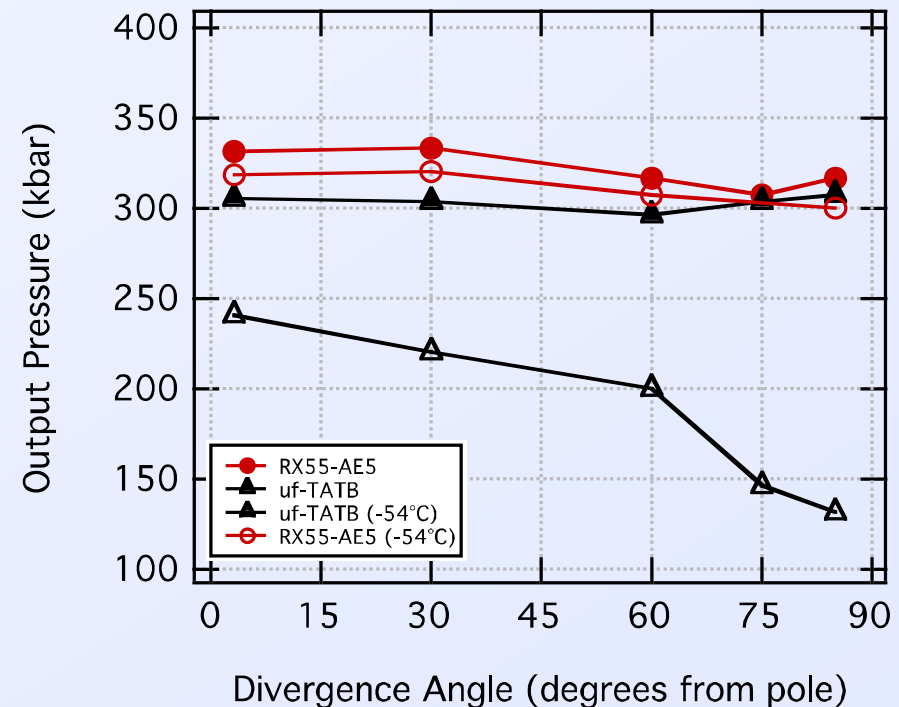
# LLM-105 formulations have shown nearly temperature-invariant booster performance.



## Breakout Timing Profiles



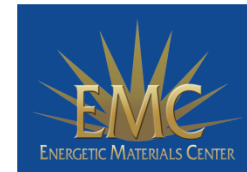
## Breakout Pressure Profiles



# LLM-105 formulations has been limited by the synthesis and manufacturing considerations

- The changing synthesis and manufacturing paths have led to a variety of research formulations being developed at LLNL.
- The original synthesis route used dimethoxy pyrazine (DMP) as a starting reagent.
- This route has been refined to increase yields, and reduce impurities and costs.
- The DMP route produces high quality crystals of modest (40-50  $\mu\text{m}$ ) mean size.
- However, this route also yields 5-10% ANPZ (2,6-diamino-3,5-dinitropyrazine), a co-product having lower density (1.800 g/cc) and less energy than LLM-105.
- A second route was developed recently that uses significantly less expensive starting reagents to produce a stable intermediate, DAPO (2,6-diamino-pyrazine-1-oxide).
- This intermediate is a non-explosive that can be manufactured in quantity and nitrated in a single step in a separate, controlled process.
- This results in a safer, and less costly manufacturing path.
- The new synthesis yields a very pure product with good yield.

# Composition, synthesis route and particle description used for each formulation discussed in this talk



**Table 1: Formulation Matrix for LLM-105-based PBX's**

Formulation	Binder	Wt. Pct. Binder	Synthesis	Crystal Mix	Density g/cc	Experiment
RX-55-AB	KelF-800	7.6	DMP	monomodal	1.825	Cylinder
RX-55-AY	Viton-A	6	DMP	bimodal	1.832	DAX
RX-55-BI	Viton-A	6	DMP	bimodal	1.818	DAX
RX-55-BJ	Viton-A	6	DAPO	monomodal	1.818	DAX
RX-55-BK	Viton-A	6	DMP	bimodal	1.818	DAX
RX-55-BP	FK-800	5	DAPO	monomodal	1.859	DAX
RX-55-BS (LX-21)	FK-800	5	DAPO	monomodal	1.861	Cylinder
RX-55-BT	Viton-A	6	DMP	bimodal	1.833	DAX
RX-55-DC (LX-22)	Viton-A	6	DMP	bimodal	1.833	Cylinder



# To provide a self-consistent detonation model we use coupled thermo-chemistry and 3D ALE codes

## ALE Hydrodynamics



## Chemistry

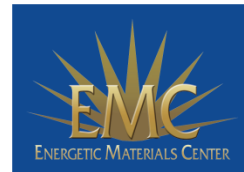
- Time advances  $\rho$  and  $E$ .
- Does spatial transport of chemical mass fractions.
- For non-ideal explosives use Cheetah as a Reactive Flow Model.

- Multi-phase first principle based EOS.
- Calculates  $P$ ,  $T$ , sound speed and other thermodynamic quantities such as thermal conduction coefficients.
- Maintains 2D and sparse multi-dimensional EOS databases.
- Solves kinetic rate equations for time evolution of chemical mass fractions.

We term our model chemistry resolved kinetic flow as Cheetah tracks the time dependent concentrations of individual species in the detonation wave and calculates EOS values based on the concentrations.

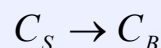
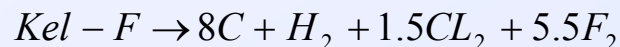
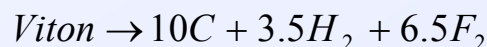
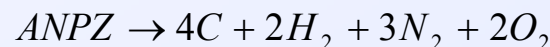
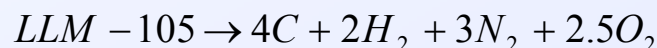


# Our Cheetah LLM-105 reactive flow model is based upon chemical composition so that it can treat all RX-55 formulations



- We have developed a Cheetah reactive flow model that can treat all LLM-105 formulations by using separate kinetic rates for each species composing the explosive.
- As LLM-105 is the dominant component we assumed that the kinetic burn rates of all initial material components are the same so all initial species burn simultaneously to products.
- We used an updated Cheetah EOS library that includes dipole effects and a LLM-105 unreacted EOS based of Riad Manaa's theoretical calculations.

## The kinetic reactions treated



$$\frac{d\lambda}{dt} = A(1-\lambda)^B (P+Q)^C$$

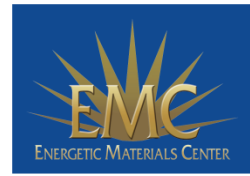
$$\frac{d\lambda}{dt} = 0 \text{ if } P+Q < 10 \text{ GPa and } \lambda < 0.1$$

$$\frac{dC_B}{dt} = EC_s e^{-T_c^*/T}$$

- The rate controlled species were LLM-105, ANPZ, Viton, Kel-F, and  $C_B$



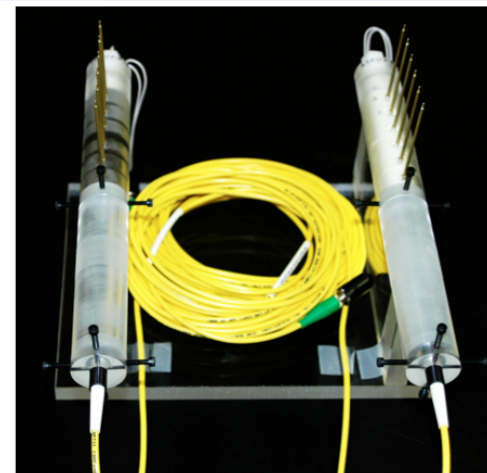
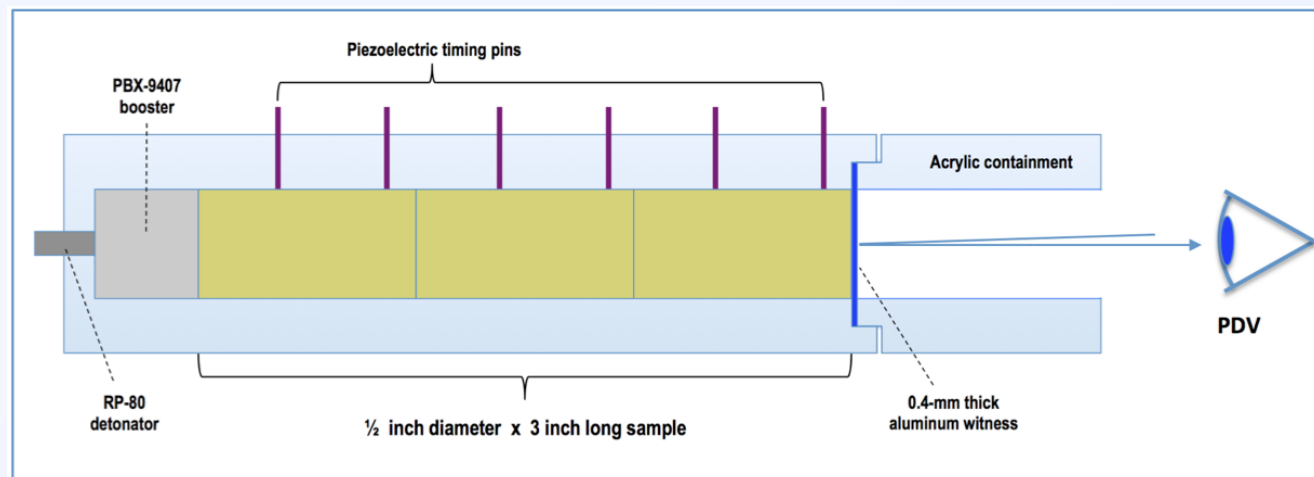
# Model calibration was based upon DAX and copper cylinder data



- Our model calibration was done using Disc Acceleration eXperiment (DAX) and copper cylinder data (detonation velocity, wall velocity, and breakout timing)
- For the LLM-105 based explosives considered here the estimated detonation reaction zone was  $\sim 0.1$  mm, which was comparable to the DAX foil thickness.
- The DAX foil velocity was primarily sensitive to detonation wave pressures close to detonation wave front.
- Copper cylinder side wall expansion experiments treat acceleration over tens of microseconds.
- This longer acceleration time scale makes the cylinder wall velocity weakly dependent upon the pressure variations within reaction zone and sensitive to the late time adiabatic regime of the detonation wave.
- The data from these two different experiments are thus complementary in being sensitive to different regions of the detonation wave.

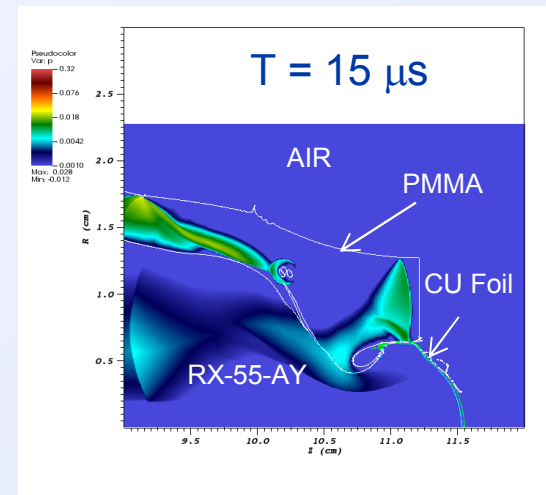
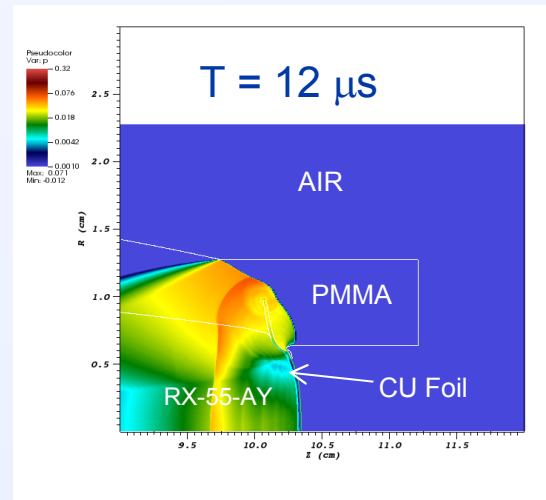
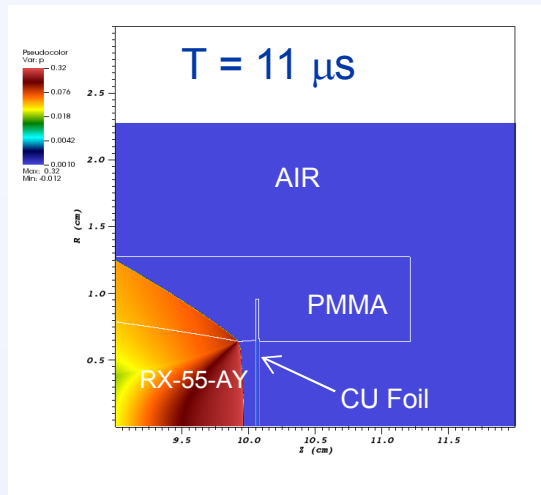
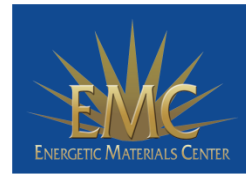


# The DAX foil velocity experiment gives a sensitive measurement detonation wave pressures close to detonation wave front.



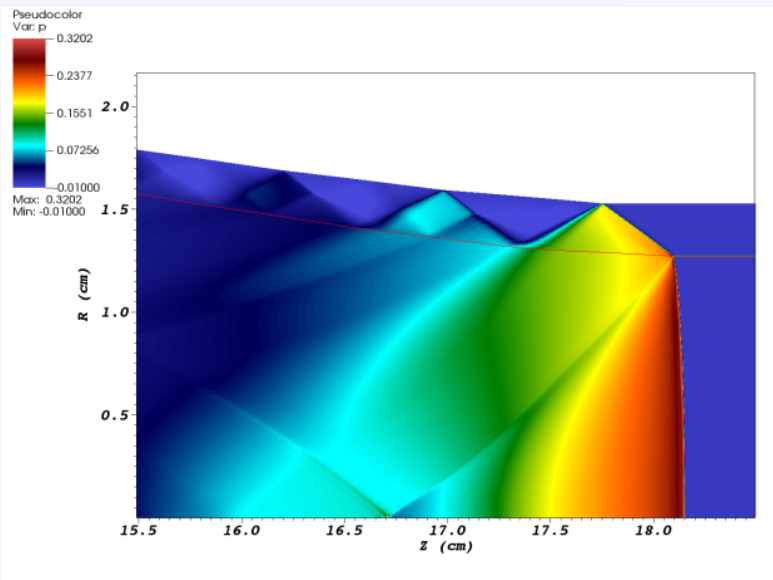
- The Disc Acceleration eXperiment (DAX) was designed to be an efficient screening tool.
  - < 20 g of sample material per shot
  - < \$5k per shot
  - High throughput: 4-8 shots per day
- Good sensitivity and precision measurement of early time detonation wave properties.

# Cheetah RX-55-AY DAX simulation results show the rapid decoupling of the foil from the HE

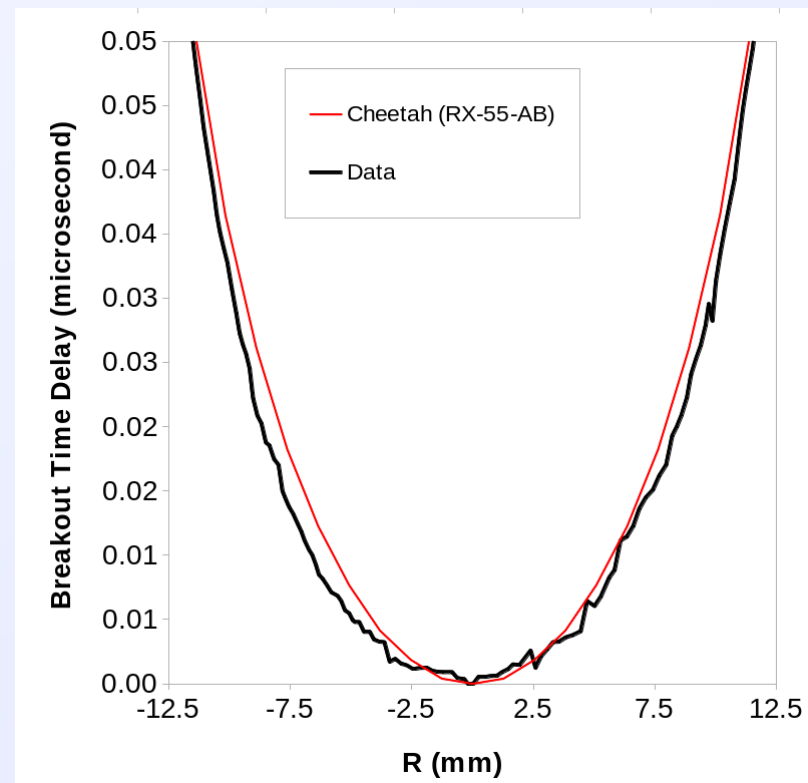


# Breakout timing for the RX-55-AB one inch diameter copper cylinder was used to calibrate our rate model

Simulation copper cylinder pressure profile showing how slight the detonation wave curvature is

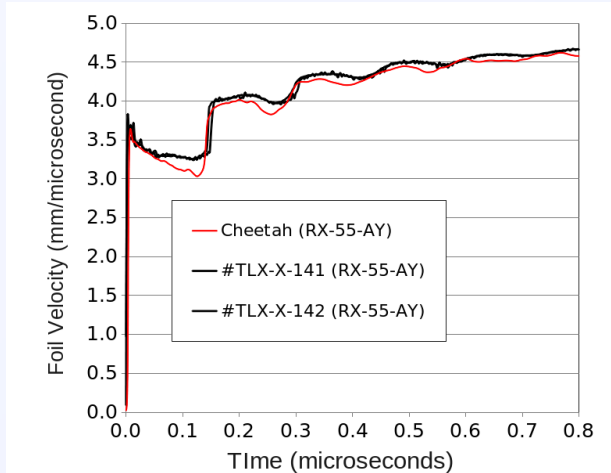


Comparison between breakout timing from simulation and data.

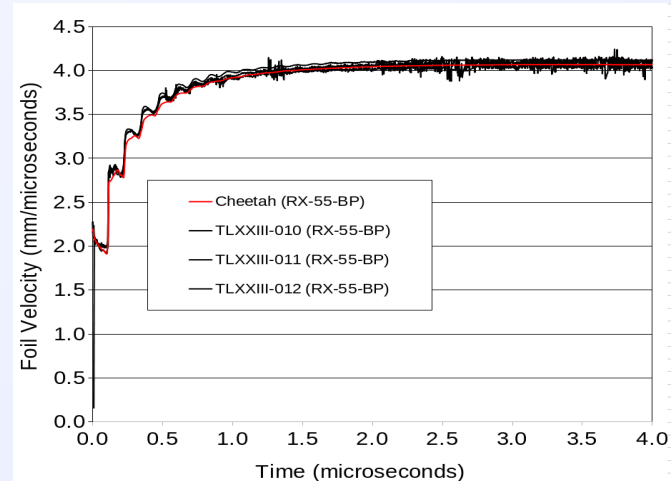


# Simulation results agree with LLM-105 data for different flyers, binders, densities, and time scales

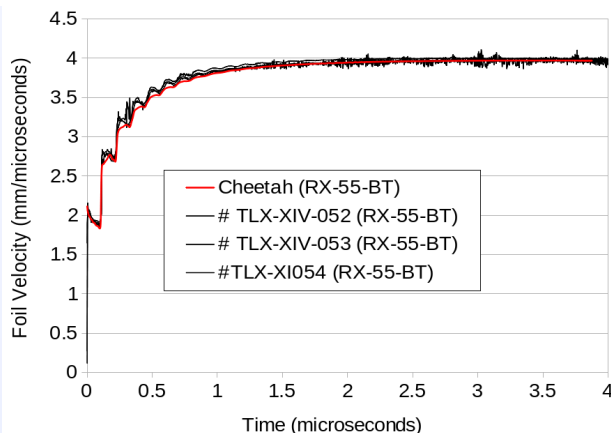
**Al Foil DAX / Viton binder / 1.832 g/cc**



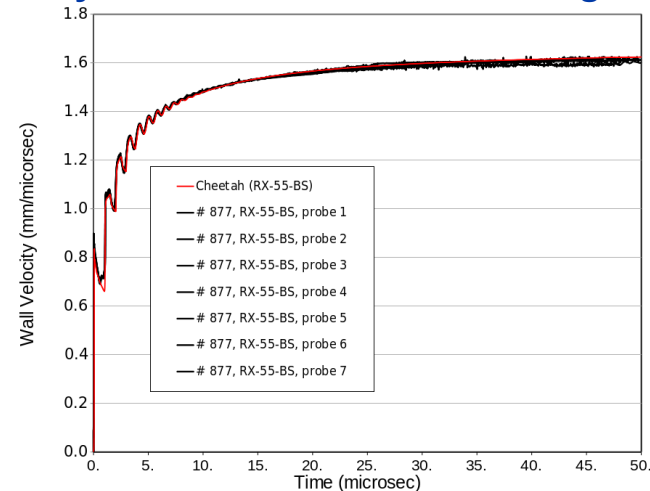
**Cu Foil DAX / Kel-F binder / 1.859 g/cc**



**Cu Foil DAX / Viton binder / 1.833 g/cc**

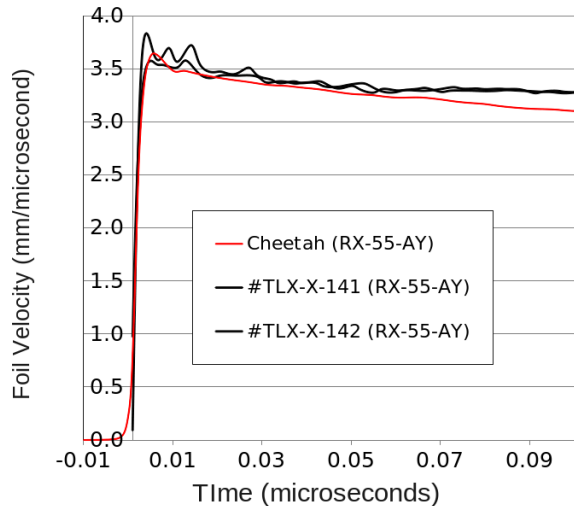


**Cu cylinder / Kel-F binder / 1.861 g/cc**

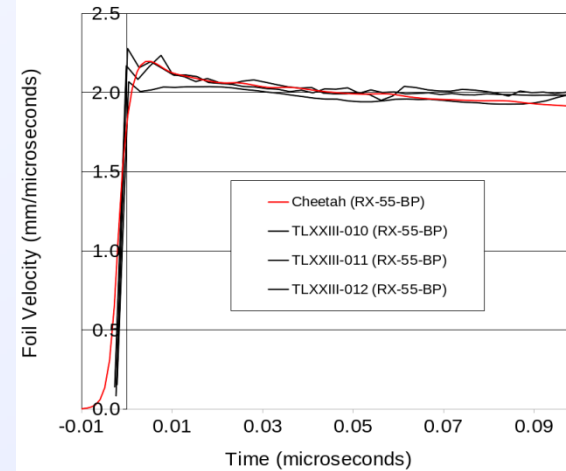


# Simulation jump-offs agree with LLM-105 data for different flyers, binders, densities, and time scales

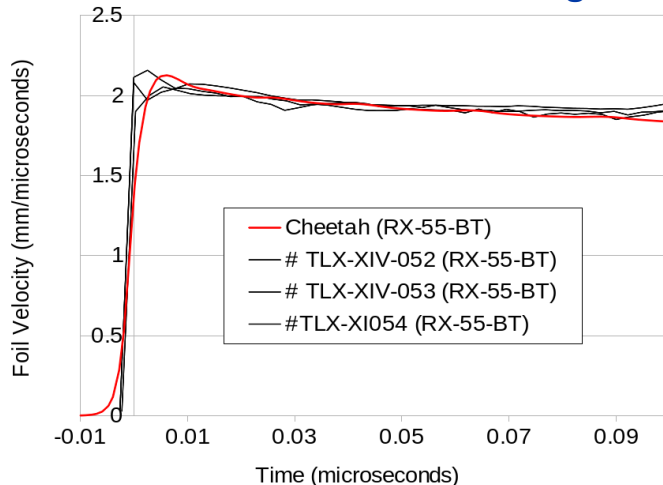
**Al Foil DAX / Viton binder / 1.832 g/cc**



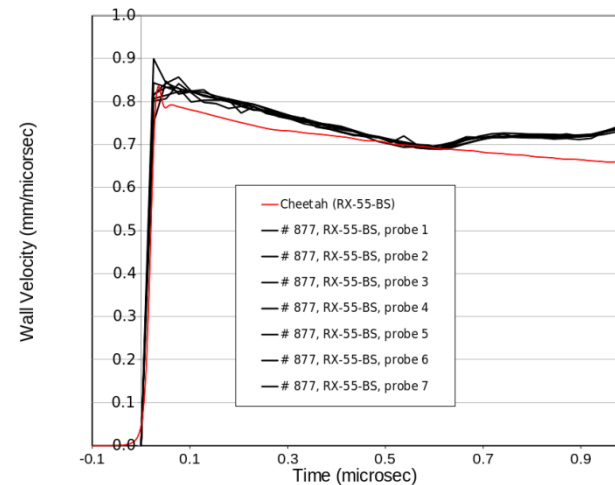
**Cu Foil DAX / Kel-F binder / 1.859 g/cc**



**Cu Foil DAX / Viton binder / 1.833 g/cc**



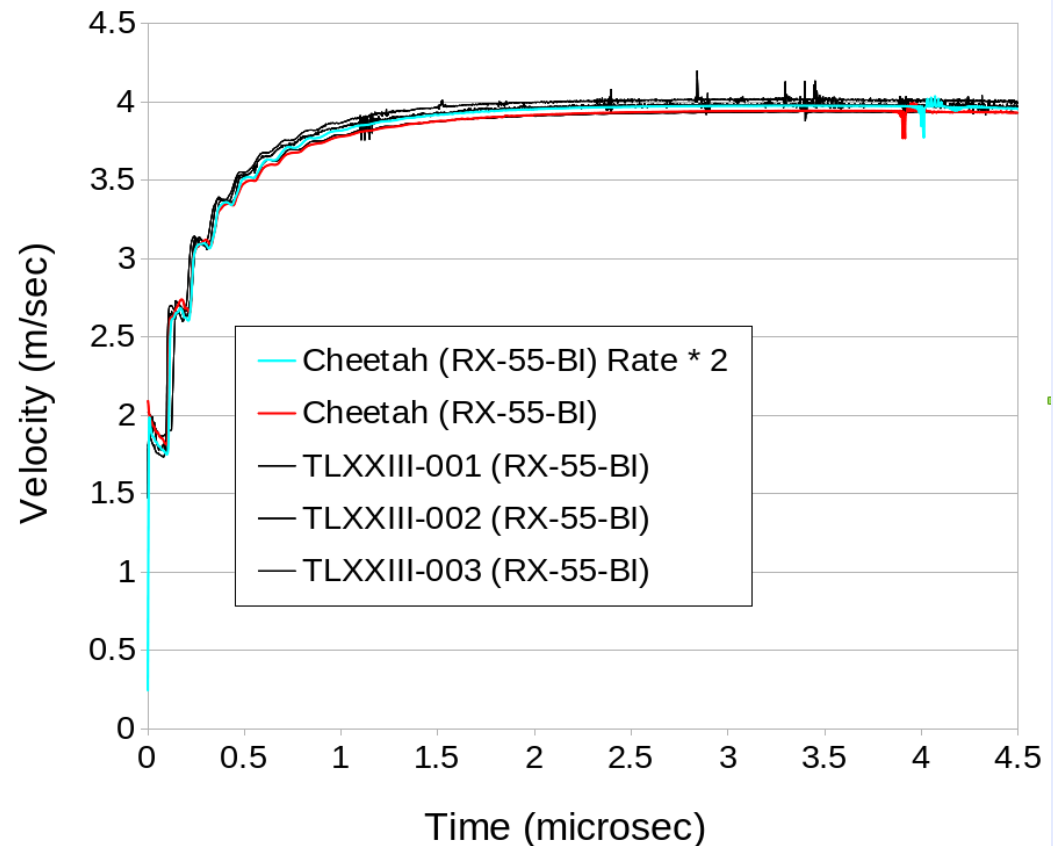
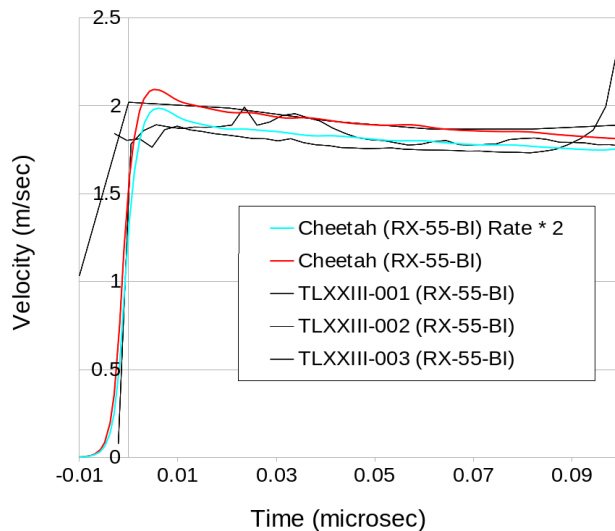
**Cu cylinder / Kel-F binder / 1.861 g/cc**



# There is evidence from DAX experiments of the burn rate increasing at low densities

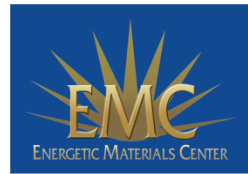
- Burn rates are likely to increase with decreasing density due to increased porosity.
- Doubling the burn rate gives better agreement with data.

Cu Foil DAX / Viton binder / 1.818 g/cc

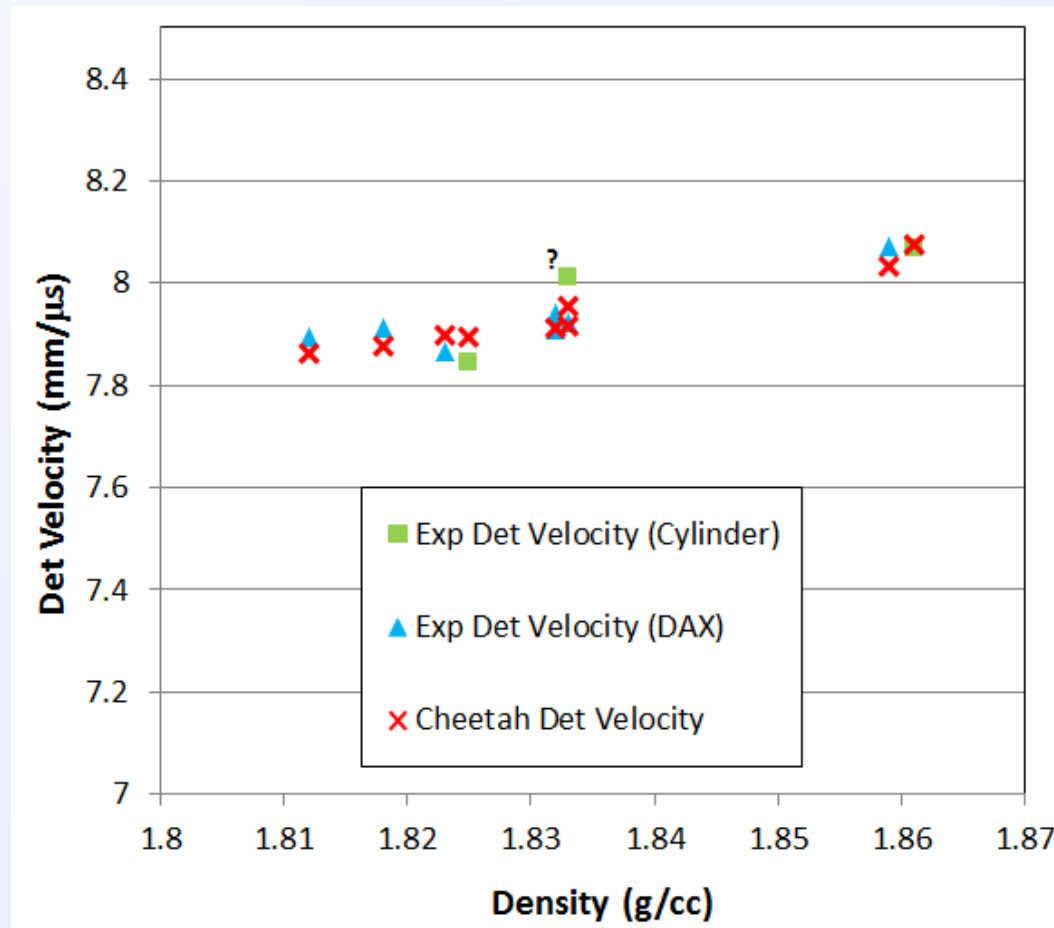




# Experimental and Cheetah detonation velocities for LLM-105 based explosives



These experimental detonation velocities are not expected to be monotonic with density as different binders are used, and the binder concentration varies from 5% to 7.6%.



# Conclusions

- We have shown here how chemistry based modeling for LLM-105 base explosives can be used to treat the different formulations, binders, densities, and time scales.
- After calibration we were able to model the LLX-105 experiments by simply specifying the initial mass fractions and initial density of each explosive.
- Good agreement is evident over a density range of 1.818-1.861 g/cc and for both Viton and Kel-F binders.
- Our Cheetah model agrees well with breakout timing, short time scale DAX foil acceleration, and long time scale copper cylinder wall acceleration.
- We plan on using this model to predict sensitivity to density, contaminants, and binders for new experiments using LLM-105 based explosives